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Density matrix based methods for bonded and non-bonded interactions

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The postulates of quantum mechanics state that the wave function contains all the possible information about a molecular system. As a consequence, all information about any bonded and non-bonded interaction a system contains or engages in should be derivable from the wave function.

In my tutorial style presentation, I will show how from the first and second order density matrices obtained from any level of theory one can obtain bond indices[1] reflecting the strength of both bonds and non-bonded interactions and how these are connected to the existence of so-called Fermi Holes and domain averaged Fermi hole analysis.[2]

[1] P. Bultinck, R. Ponec, S. Van Damme, "Multicenter Bond Indices as a New Measure of Aromaticity in Polycyclic Aromatic Hydrocarbons" J. Phys. Org. Chem., 18 (2005) 706-718.
[2] P. Bultinck, D.L. Cooper, D.L., R. Ponec, "The influence of atoms-in-molecules methods on shared-electron distribution indices and domain averaged Fermi Holes" J. Phys. Chem. A, Published online, 2010. DOI: 10.1021/jp101707w.